REPORT DOCUMENTATION PAGE

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Approved for public release; distribution unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT

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15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Leilani Richardson
Unclassified	Unclassified	Unclassified	A		19b. TELEPHONE NUMBER *(include area code)* (661) 275-5015

62 separate items are enclosed

C8

MEMORANDUM FOR PRS (Contractor/In-House Publication)

FROM: PROI (TI) (STINFO) 26 September 2000

SUBJECT: Authorization for Release of Technical Information, Control Number: **AFRL-PR-ED-AB-2000-181**
Christe, K.O. (ERC); Vij, Ashwani; Mews, R.; Zhang, X. (USC), Boatz, J. (PRSP), "Method for Solving Some Disordered Crystal Structures and its Application to the Structures of NF2O+ and SO2F-"
(Oral Presentation)

15th Winter Fluorine Conference (St. Petersberg, FL, 14 Jan 2001) **(Statement A)**
(Past Deadline: 14 Sep 2000)

1. This request has been reviewed by the Foreign Disclosure Office for: a.) appropriateness of distribution statement, b.) military/national critical technology, c.) export controls or distribution restrictions, d.) appropriateness for release to a foreign nation, and e.) technical sensitivity and/or economic sensitivity.
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PHILIP A. KESSEL Date
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METHOD FOR SOLVING SOME DISORDERED CRYSTAL STRUCTURES AND ITS APPLICATION TO THE STRUCTURES OF NF2O+ AND SO2F-. **Karl O. Christe,** Ashwani Vij, Rudiger Mews, Xiongzhi Zhang, Jerry Boatz., Air Force Research Laboratory, Edwards AFB, CA 93524 and University of Southern California, Los Angeles, CA 90089, University of Bremen, Bremen, Germany.

Oxygen and fluorine ligands are similar in size and frequently exhibit positional disorder in the crystal structures of oxofluorides, resulting in a partial or complete averaging of the observed bond lengths and angles. The failure to recognize the presence of disorder has resulted in the publication of numerous incorrect structures, while the recognition of disorder problems has generally prompted researchers to abandon these data sets. In this paper, a method is outlined which allows in favorable cases the extraction of the correct individual bond lengths and angles from disordered data. The method is demonstrated for the SO2F- and NOF2+ ions, and the correctness of the derived bond lengths is supported by ab initio calculations for the free ions.

ABSTRACT. Please be BRIEF—150 words maximum if possible. Title of paper should be ALL CAPS; author(s) listed by first name, middle initial, last name; indicate address with zip code.

A. DIVISION OF FLUO Division Member ☒ Yes ☐ No

B. ACS MEMBER ☒ Yes ☐ No

(To be filled in by Division)
Paper number as listed on program _____

C. TITLE OF PAPER Method for solving some disordered crystal structures and its application to the structures of NF2O+ and SO2F-

Please indicate preference: ☒ Oral ☐ Poster
☐ withdraw if oral/poster format cannot be met

D. AUTHORS

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G. For contributed papers, do authors meet criteria outline in ACS Bylaw VI, Section 6(3)? See instructions.

☐ Yes ☐ No

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